

Education

- 2017-2021 **National University of Science and Technology MISIS - Bachelor's Degree**
Materials Science Department
- 2021-2023 **Skolkovo Institute of Science and Technology - Master's Degree**
Materials Science Department
- 2023-present **Skolkovo Institute of Science and Technology - PhD**
Materials Science Department

Current position

- 2022-Present **Department of Light-Induced Surface Phenomena, Prokhorov General Physics Institute of the Russian Academy of Sciences**
Grant participant (grant № 22-22-00555)
- 2023-Present **Skolkovo Institute of Science and Technology - research intern**
MDL laboratory

Experience

- 2017-2019 **Laboratory of X-ray Structural Research and Diagnostics of Materials, NUST MISIS**
Research on properties and structure of amorphous material using various methods
- 2020-2022 **Laboratory of the Theory of Superconductivity and Statistical Physics of Complex Systems, Lebedev Physical Institute**
Global optimization structure of nanoclusters (Cu-Au, Pt-Pd) using GUPTA Potential, DFT calculations
- 2020-Present **Computational Materials Discovery Laboratory, Skoltech**
Structure and stability of nanoclusters promising for catalysis. (Catalytic activity of Cu-Au nanoclusters for CO oxidation)
- 2023 - Present **Department of Chemical and Biomolecular Engineering, Computational Nanocatalysis, National University of Singapore**
The effect of adsorbant concentration on the catalytic properties of nanoclusters

Internships

- 2022 Industrial Immersion in "Core Technologies"
- 2023 Department of Chemical and Biomolecular Engineering, Computational Nanocatalysis, National University of Singapore

Courses

- 2020 19th ONLINE USPEX workshop (19th Lyakhov school) - participant
- 2020 Online course "From structure to production: Methods and approaches to predicting and obtaining new materials with high performance" - participant

Conferences

- 2022 Workshop "Modern trends in Computational Materials Discovery",
Isfahan University of Technology - tutor and poster presenter

Publications

Dmitry V. Rybkovskiy, Sergey V. Lepeshkin, Vladimir S. Baturin, Anastasiia A. Mikhailova and Artem R. Oganov "Phosphorus nanoclusters and insight into the formation of phosphorus allotropes", *Nanoscale*, 15, 1338-1346 (2023).

DOI: 10.1039/D2NR06523A, Impact factor 8.307 Q1

Anastasiia A. Mikhailova, Sergey V. Lepeshkin, Vladimir S. Baturin, Alexey P. Maltsev, Yurii A. Uspenskii, and Artem R. Oganov "Ultralow reaction barriers for CO oxidation in Cu–Au nanoclusters", *Nanoscale*, 2023, DOI: 10.1039/D3NR02044D, Impact factor 8.307 Q1

Skills

English (upper-intermediate)

Python (visualisation and data analysis), Linux

Familiar Packages: Gaussian, VASP, LAMMPS, USPEX, MLIP, MOPAC

Research interests

nanoclusters in gas phase and on a substrate
surfaces

structure prediction algorithm

molecular dynamic simulation

ab initio calculations

prediction of reaction mechanism

calculation of reaction barriers